Does the Hubbard Model Show $d_{x^2-y^2}$ Superconductivity?

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Abstract

It is rigorously shown that the two-dimensional Hubbard model with narrow bands (including next nearest-neighbor hopping, etc.) does not exhibit $d_{x^2-y^2}$-wave pairing long-range order at any nonzero temperature. This kind of pairing long-range order will also be excluded at zero temperature if an excited energy gap opens in the charge excitation spectrum of the system. These results hold true for both repulsive and attractive Coulomb interactions and for any electron fillings, and are consistent with quantum Monto Carlo calculations.

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Considerable experimental evidence shows that the dominant symmetry of the pairing order parameter in high temperature superconductors may be $d_{x^2-y^2}$-wave (see, e.g., Ref. [1] for a review). Though some disputes [2] regarding this challenging issue still remain, a great number of people arrive at such a consensus that exploring the possibility of d-wave superconductivity in strongly correlated electrons would be quite useful towards ultimately successfully explaining high temperature superconductivity, thus resulting in numerous studies on this subject. As a matter of fact, owing to its apparent simplicity the two-dimensional (2D) Hubbard model naturally becomes an actively debating focus in recent years, as it is widely thought to provide a simple model to interpret some essential features relevant to the physical properties of CuO_2 planes in the cuprate oxides. In spite of intense efforts being made both numerically and analytically [3,4], however, a basic question whether or not the $d_{x^2-y^2}$-wave pairing long-range order (LRO) in the 2D Hubbard model exists, is still inconclusive. Actually, at energy scales and lattice sizes accessible to numerical simulations no definite sign of $d_{x^2-y^2}$ superconductivity has been detected in this model, while some analytical works using different approximations appear to suggest positive answers [3–5], thereby leaving some controversies and ambiguities to be resolved. To clarify them, rigorous results are particularly needed at this stage.

In this paper, based on Bogoliubov's inequality we show rigorously that the 2D Hubbard model with narrow bands (including next nearest-neighbor hopping, etc.) does not exhibit $d_{x^2-y^2}$-wave pairing LRO at any nonzero temperature. This kind of pairing LRO will also be excluded if a gap opens in the charge excitation spectrum of the system. These results hold true for both repulsive and attractive Coulomb interactions and for any electron fillings. Combining with other known exact results, one would conclude that the 2D Hubbard model might not have the right stuff for describing superconductivity in the cuprate oxides in this sense provided that the superconducting mechanisms in these materials are supposed to be due to condensation of either s-wave Cooper, or generalized η or $d_{x^2-y^2}$-wave electron pairs. The present observations are consistent with quantum Monto Carlo results.

Let us start with some preliminary definitions. The $d_{x^2-y^2}$-wave pairing operator (like

the Cooper pairing operator) can be defined as [6]

$$\Delta_d^+ = \sum_{\mathbf{k}} (\cos k_x - \cos k_y) c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger = \frac{1}{2} \sum_{\mathbf{r},\boldsymbol{\delta}} f(\boldsymbol{\delta}) c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}+\boldsymbol{\delta}\downarrow}^\dagger, \quad \Delta_d^- = (\Delta_d^+)^\dagger, \tag{1}$$

where we have used the Fourier transform of an electron operator $c_{\mathbf{k}\sigma}$

$$c_{\mathbf{k}\sigma} = \frac{1}{\sqrt{M}} \sum_j \exp(i\mathbf{k}\cdot\mathbf{R}_j) c_{j\sigma}, \quad c_{j\sigma} = \frac{1}{\sqrt{M}} \sum_{\mathbf{k}} \exp(-i\mathbf{k}\cdot\mathbf{R}_j) c_{\mathbf{k}\sigma}, \tag{2}$$

and $f(\boldsymbol{\delta}) = +1$ (-1) for $\boldsymbol{\delta} = \pm\mathbf{a}_x$ $(\pm\mathbf{a}_y)$, and zero otherwise, where $\mathbf{a}_x$, $\mathbf{a}_y$ are unit vectors connecting nearest-neighbor sites, M is the number of lattice sites, $\mathbf{R}_j$ $(\mathbf{r})$ is the position vector of jth (rth) site, and σ denotes spin. In the following we for simplicity take $\boldsymbol{\delta} = \pm\mathbf{a}_x$, $\pm\mathbf{a}_y$. According to Bogoliubov [7], when one studies a degenerate state of the statistical equilibrium, one should first remove the degeneracy by introducing a symmetry-breaking field, and then turn to investigate the so-called quasi-averages involved. On account of this reason we define the $d_{x^2-y^2}$-wave pairing order parameter per site as

$$g = \lim_{\nu\to 0^+} \lim_{M\to\infty} \langle \frac{\Delta_d^+}{M} \rangle, \tag{3}$$

where $\langle\cdots\rangle$ stands for the thermal average in a grand canonical ensemble, and ν is the amplitude of a U(1) symmetry-breaking field. Note that the two limit processes are non-interchangeable. The nonvanishing of g, namely $g \neq 0$ means the existence of $d_{x^2-y^2}$-wave pairing LRO, while $g = 0$ gives the converse result.

We now consider a general Hubbard model with narrow bands on a periodic lattice in the presence of a U(1) symmetry-breaking field. The Hamiltonian reads

$$\begin{aligned} H = &\sum_{i,j} \sum_{\sigma} T(\mathbf{R}_i - \mathbf{R}_j) c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow} - \sum_i \mu_i (n_{i\uparrow} + n_{i\downarrow}) \\ &-\nu(\Delta_d^+ + \Delta_d^-), \end{aligned} \tag{4}$$

where the sum on i and j can run over all M lattice sites, $c_{i\sigma}^\dagger$ $(c_{i\sigma})$ is the creation (annihilation) operator for an electron at site i with spin σ, the on-site Coulomb interaction U_i and the chemical potential μ_i are allowed to be position-dependent for generality, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, the number operator of electrons. $T(\mathbf{R}_i - \mathbf{R}_j)$, which has a property

$T(\mathbf{R}_i - \mathbf{R}_j) = T^*(\mathbf{R}_j - \mathbf{R}_i)$, is the local overlap integral which designates the energy bands of the model. In fact we require that $T(\mathbf{R}_i - \mathbf{R}_j)$ survives only for short-r anged overlapping in the present case. The last term in Eq.(4) introduces the effect of the U(1) symmetry-breaking field, where ν is an infinitesimal quantity, and $\Delta_d^{\pm}$ are given by Eq.(1).

As we attempt to explore the possibility of $d_{x^2-y^2}$ pairing LRO in Eq.(4), in the following we shall use Bogoliubov's inequality [8,9]

$$|\langle [C^\dagger, A^\dagger] \rangle|^2 \leq \frac{\beta}{2} \langle \{A, A^\dagger\} \rangle \langle [[C, H], C^\dagger] \rangle, \tag{5}$$

for any quantum-mechanical operators A and C, and with the inverse temperature $\beta = 1/T$ ($k_B = 1$), where $[,]$ and $\{,\}$ are the usual commutator and anticommutator, respectively. This inequality was used to exclude the possibility of magnetic LRO in the Heisenberg [9] and Hubbard [10,11] models as well as superfluidity in Fermi liquids [12] in one and two dimensions at nonzero temperature. Quite recently, this inequality was also used to exclude the possibility of s-wave Cooper pairing and generalized η pairing LRO in the 1D and 2D Hubbard models with narrow bands at nonzero temperature [13]. It should be mentioned that the SU(2) Lie algebra obeyed by the relevant operators (e.g., spin operators, Cooper pairing operators and η pairing operators, etc.) plays a key role in applying this inequality to the above-mentioned cases. However, one may observe that the $d_{x^2-y^2}$-wave pairing operators defined in Eq.(1) do not obey the SU(2) symmetry, which makes Bogoliubov's inequality not directly applicable to the present case, as stated in Ref. [13]. Fortunately, this difficulty can be overcome by noting the simple fact that $f(\boldsymbol{\delta})$ in Eq.(1) takes values either $+1$ and -1 or zero so that we can decompose the $d_{x^2-y^2}$ pairing order parameter per site, g, into four terms each of which obeys the SU(2) algebra. It is this property that makes it possible for applying inequality (5) to our case [14]. We would like to mention here that although one can find the standard derivations in Refs. [9–11,13], for reader's convenience and for this paper being self-contained, we shall below intend to present our calculations in some detail.

We define the following operators

$$\tilde{\eta}^{+}_{\mathbf{r}} = c^{\dagger}_{\mathbf{r}\uparrow} c^{\dagger}_{\mathbf{r}+\boldsymbol{\alpha}\downarrow}, \quad \tilde{\eta}^{-}_{\mathbf{r}} = c_{\mathbf{r}+\boldsymbol{\alpha}\downarrow} c_{\mathbf{r}\uparrow}, \quad \tilde{\eta}^{z}_{\mathbf{r}} = \frac{1}{2}(n_{\mathbf{r}\uparrow} + n_{\mathbf{r}+\boldsymbol{\alpha}\downarrow} - 1), \tag{6}$$

with an arbitrary constant vector $\boldsymbol{\alpha}$ on the lattice. It can be verified that they satisfy

$$[\tilde{\eta}^{+}_{\mathbf{r}}, \tilde{\eta}^{-}_{\mathbf{r}'}] = 2\tilde{\eta}^{z}_{\mathbf{r}} \delta_{\mathbf{r}\mathbf{r}'}, \qquad [\tilde{\eta}^{\pm}_{\mathbf{r}}, \tilde{\eta}^{z}_{\mathbf{r}'}] = \mp \tilde{\eta}^{\pm}_{\mathbf{r}} \delta_{\mathbf{r}\mathbf{r}'}. \tag{7}$$

The Fourier transforms of $\tilde{\eta}$ operators, like spin operators in Refs. [9,11], are defined by

$$\tilde{\eta}^{\pm,z}_{\mathbf{r}} = \frac{1}{M} \sum_{\mathbf{k}} \exp(-i\mathbf{k}\cdot\mathbf{r}) \tilde{\eta}^{\pm,z}(\mathbf{k}), \qquad \tilde{\eta}^{\pm,z}(\mathbf{k}) = \sum_{\mathbf{r}} \exp(i\mathbf{k}\cdot\mathbf{r}) \tilde{\eta}^{\pm,z}_{\mathbf{r}}, \tag{8}$$

which comply

$$[\tilde{\eta}^{+}(\mathbf{k}), \tilde{\eta}^{-}(\mathbf{k}')] = 2\tilde{\eta}^{z}(\mathbf{k}+\mathbf{k}'), \quad [\tilde{\eta}^{\pm}(\mathbf{k}), \tilde{\eta}^{z}(\mathbf{k}')] = \mp \tilde{\eta}^{\pm}(\mathbf{k}+\mathbf{k}'). \tag{9}$$

Eqs.(9) come from Eqs.(7) and (8).

With these definitions we choose $A = \tilde{\eta}^{+}(-\mathbf{k}-\mathbf{Q})$ and $C = \tilde{\eta}^{z}(\mathbf{k})$ in (5) for our purposes. After some algebra for the double-commutator one gets the inequality,

$$\begin{aligned} \langle [[\tilde{\eta}^{z}(\mathbf{k}), H], \tilde{\eta}^{z}(-\mathbf{k})] \rangle \le \frac{1}{2} \sum_{i} |T(\mathbf{R}_i)| |\cos(\mathbf{k}\cdot\mathbf{R}_i) - 1| &\Big| \sum_{\mathbf{k}'\sigma} e^{i\mathbf{k}'\cdot\mathbf{R}_i} \langle c^{\dagger}_{\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma} \rangle \Big| \\ + |\nu| |\langle \Delta^{+}_{d} + \Delta^{-}_{d} \rangle| & \\ \le \frac{N}{4} \sum_{i} |T(\mathbf{R}_i)| R_i^2 k^2 + 2|\nu| \cdot |\langle \Delta^{+}_{d} \rangle|. & \end{aligned} \tag{10}$$

In the derivation of this inequality we have used the property of translation invariance and such a few simple facts as $\sum_{\mathbf{k}'\sigma} \langle c^{\dagger}_{\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma} \rangle = N$, the total number of electrons, $1 - \cos x < x^2/2$ and $\langle \Delta^{+}_{d} \rangle = \langle \Delta^{-}_{d} \rangle^{\dagger}$. Substituting inequality (10) into (5) we have

$$\frac{1}{M} \langle \{ \tilde{\eta}^{+}(-\mathbf{Q}-\mathbf{k}), \tilde{\eta}^{-}(\mathbf{Q}+\mathbf{k}) \} \rangle \ge \frac{2|\mathcal{F}_{\nu,M}(\mathbf{Q},\boldsymbol{\alpha})|^2}{\beta(\xi k^2 + 2|\nu| |\langle \Delta^{+}_{d}/M \rangle|)}, \tag{11}$$

where $\mathcal{F}_{\nu,M}(\mathbf{Q},\boldsymbol{\alpha}) = \langle \tilde{\eta}^{+}(\mathbf{Q}) \rangle / M$, and $\xi = (N/M) \sum_i |T(\mathbf{R}_i)| \mathbf{R}_i^2 / 4$. Since the $T(\mathbf{R}_i)$'s are the matrix elements of the overlap integral between Wannier functions which decrease rapidly with distance for strongly correlated electrons, the summation $\sum_i |T(\mathbf{R}_i)| \mathbf{R}_i^2$ is well defined. For the single-band Hubbard model as well as one with next nearest-neighbor hopping integral the values of $\sum_i |T(\mathbf{R}_i)| \mathbf{R}_i^2$ on a hypercubic lattice can be

found in Ref. [13]. Summing both sides of the above inequality over $\mathbf{k}$ and noting that $(1/M)\sum_{\mathbf{k}}\langle\{A, A^\dagger\}\rangle = \sum_{\mathbf{r}}\langle\{\tilde{\eta}_{\mathbf{r}}^+, \tilde{\eta}_{\mathbf{r}}^-\}\rangle = \sum_{\mathbf{r}}\langle[1-(n_{\mathbf{r}\uparrow}-n_{\mathbf{r}+\boldsymbol{\alpha}\downarrow})^2]\rangle \leq M$, we obtain

$$|\mathcal{F}_{\nu,M}(\mathbf{Q},\boldsymbol{\alpha})|^2 \leq \frac{\beta M}{2}\left(\sum_{\mathbf{k}}\frac{1}{\xi k^2 + 2|\nu||\langle\Delta_d^+/M\rangle|}\right)^{-1}. \tag{12}$$

Now we take the thermodynamic limit, i.e., $N \to \infty$ and $M \to \infty$ with the ratio N/M fixed. Then the sum on $\mathbf{k}$ in (12) can be replaced by the integral over the first Brillouin zone. Suppose that k_0 is the distance of the nearest Bragg plane from the origin in $\mathbf{k}$ space. Then we obtain for small ν the following inequalities

$$|\mathcal{F}_{\nu,\infty}(\mathbf{Q},\boldsymbol{\alpha})| \leq (\xi\beta^2)^{1/4}|\nu|^{1/4}, \qquad (1D) \tag{13}$$

$$|\mathcal{F}_{\nu,\infty}(\mathbf{Q},\boldsymbol{\alpha})| \leq \sqrt{\frac{\xi\beta}{\pi}}\frac{1}{|\ln|\nu||^{1/2}}, \qquad (2D) \tag{14}$$

where we have used $\lim_{M\to\infty}|\langle\Delta_d^+/M\rangle| \leq 2$ in (13). Inequalities (13) and (14) tell us that $|\mathcal{F}_{0,\infty}(\mathbf{Q},\boldsymbol{\alpha})| = 0$ for any nonzero temperature as the U(1) symmetry-breaking field is turned off ($\nu \to 0^+$). (Recall that the thermodynamic limit has been taken before we remove the U(1) symmetry-breaking field.) This means that $\mathcal{F}_{0,\infty}(\mathbf{Q},\boldsymbol{\alpha}) := \lim_{\nu\to 0^+}\lim_{M\to\infty}\langle(1/M)\sum_{\mathbf{r}}\exp(i\mathbf{Q}\cdot\mathbf{r})c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}+\boldsymbol{\alpha}\downarrow}^\dagger\rangle_{\nu,M} = 0$ for *any* possible $\mathbf{Q}$ and $\boldsymbol{\alpha}$ for $T > 0$ in the 1D and 2D Hubbard models defined in Eq.(4). On the other hand, we note that the $d_{x^2-y^2}$-wave pairing order parameter per site can be rewritten as $g = (1/2)\sum_{\boldsymbol{\delta}} f(\boldsymbol{\delta})\mathcal{F}_{0,\infty}(\mathbf{0},\boldsymbol{\delta})$ because the existence of $\mathcal{F}_{0,\infty}(\mathbf{0},\boldsymbol{\delta})$ has been proved, where we have set $\mathbf{Q} = \mathbf{0}$ and $\boldsymbol{\alpha} = \boldsymbol{\delta}$. Here use has been made of the well-known theorem: $\lim a \pm \lim b = \lim(a \pm b)$ if $\lim a$ and $\lim b$ exist. Since $\mathcal{F}_{0,\infty}(\mathbf{0},\boldsymbol{\delta}) = 0$ for $T > 0$ and $f(\boldsymbol{\delta})$, by virtue of its definition, takes either ± 1 or zero, we finally have $g = 0$ for $T > 0$. Consequently, we have proved that the 2D Hubbard model with narrow bands, defined by Eq.(4), does not show $d_{x^2-y^2}$-wave pairing LRO at any nonzero temperature.

When $\beta/2$ is replaced by $1/E_{gap}$ in inequality (5), where E_{gap} (> 0) is an excitation energy gap between the lowest excited state and the ground state of the system, (5) still holds true at zero temperature. We refer to Refs. [13,15] for detail discussions. Therefore, all the above analyses can apply to the case at zero temperature except $\beta/2$ replaced by $1/E_{gap}$.

Then we could conclude that if an energy gap opens in the charge excitation spectrum of the system (4), there will also be no $d_{x^2-y^2}$-wave pairing LRO in two dimensions at zero temperature.

A few remarks are in order. (i) The derivations above presented are valid for both repulsive and attractive on-site Coulomb interactions and for any electron filling fraction. (ii) The method used in this paper can be readily extended to exclude the possibility of extended s-wave [with pairing operator $\Delta^+_{e-s} = \sum_{\mathbf{k}}(\cos k_x + \cos k_y)c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}$] superconductivity in the 1D and 2D Hubbard models at finite temperatures. In the Hilbert subspace without doubly-occupied sites this method might be applied to the t-J model as well. It should be emphazied that the method works only for low dimensions (1D and 2D), not for three dimensions. (iii) The conclusions drawn in this paper are quite consistent with the results from numerical simulations (e.g., quantum Monte Carlo calculations) in the 2D Hubbard model. We refer to Refs. [3–5] for excellent reviews. The practical situation is that although most numerical works show some tendencies favouring $d_{x^2-y^2}$ superconductivity, but no definite sign of LRO has been detected, as pointed out in Refs. [16,17]. We would like to mention here that the present conclusions are not incompatible with the quantum Monte Carlo observations that the long-tailed enhancements in the $d_{x^2-y^2}$ pairing correlation near half-filling [17] or the exhibition of $d_{x^2-y^2}$-like pairing fluctuations at low temperatures [18] are detected in the 2D Hubbard model. Recent analytic and quantum Monte Carlo results also show that the 2D Hubbard model with next nearest-neighbor hopping integral does not exhibit any definite sign of s-wave and d-wave superconductivity [19–22], consistent with the present exact result. (iv) The nonexistence of s-wave Cooper pairing and generalized η pairing LRO at finite temperatures in the 1D and 2D Hubbard models with narrow bands has been proved in Ref. [13,23]. Combining these exact results one would conclude that the 2D Hubbard model might not have the right stuff for explaining high temperature superconductivity in the layered cuprate oxides if the superconducting mechanisms in these materials are supposed to be due to condensation of one of the above-mentioned electron pairs, as a successful t heory should describe unifyingly the properties not only at zero

temperature but also at finite temperatures. (v) To choose a proper model which could exhibit $d_{x^2-y^2}$-wave pairing LRO in 2D, one may consider those which contain electron interactions not commuting with the operator $\sum_{\mathbf{r}} \exp(i\mathbf{k}\cdot\mathbf{r}) n_{\mathbf{r}}$, like one investigated in Ref. [16], because in this way Bogoliubov's inequality becomes ineffective. Another possibility is that the coupling between layers in the cuprate oxides might ought to be considered, which could also make Bogoliubov's inequality ineffective.

To summarize, we show rigorously that, by means of Bogoliubov's inequality, the 2D Hubbard model with narrow bands (including next nearest-neighbor hopping, etc.) does not exhibit $d_{x^2-y^2}$ wave pairing LRO at any nonzero temperature. This kind of pairing LRO will also be excluded if an excited energy gap opens in the charge excitation spectrum of the system. These results are valid for both repulsive and attractive Coulomb interactions and for any electron fillings. Combining with known exact results obtained previously one would conclude that the 2D Hubbard model might not have enough right stuff for describing superconductivity in the cuprate oxides if the superconducting mechanisms in these materials are supposed to be due to condensation of one of the aforementioned electron pairs. The present observations are consistent with quantum Monto Carlo results.

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